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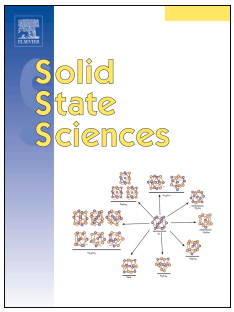

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On the novel double perovskites $A_2Fe(Mn_{0.5}W_{0.5})O_6$ (A= Ca, Sr, Ba). Structural evolution and Magnetism from Neutron Diffraction data

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To the memory of Prof. Gérard Demazeau

Abstract: New $A_2Fe(Mn_{0.5}W_{0.5})O_6$ (A= Ca, Sr, Ba) double perovskite oxides have been prepared by ceramic techniques. X-ray diffraction (XRD) complemented with neutron powder diffraction (NPD) indicate a structural evolution from monoclinic (space group $P2_1/n$) for A= Ca to cubic ($Fm\text{-}3m$) for A= Sr and finally to hexagonal ($P6_3/mmc$) for A= Ba as the perovskite tolerance factor increases with the A^{2+} ionic size. The three oxides present different tilting schemes of the FeO_6 and $(Mn,W)O_6$ octahedra. NPD data also show evidence in all cases of a considerable anti-site disordering, involving the partial occupancy of Fe positions by Mn atoms, and vice-versa. Magnetic susceptibility data show magnetic transitions below 50 K characterized by a strong irreversibility between ZFC and FC susceptibility curves. The A = Ca perovskite shows a G-type magnetic structure, with weak ordered magnetic moments due to the mentioned antisite disordering. Interesting magnetostrictive effects are observed for the Sr perovskite below 10 K.

Keywords: Double perovskite; tolerance factor; anti-site disordering; neutron diffraction; Sr_2FeMoO_6

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